

STN 1-17-03
Author Search

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS
AN 1998:142921 CAPLUS
TI Olefin trimerization with 1,3,5-triazacyclohexane complexes of chromium
AU **Koehn, R. D.; Haufe, M.**; Kociok-Koehn, G.
CS Institut f. Anorg. u. Analyt. Chemie, TU Berlin, Berlin, 10623, Germany
SO Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), INOR-278 Publisher: American Chemical Society, Washington, D. C. CODEN: 65QTAA
DT Conference; Meeting Abstract
LA English
AB Most catalytic olefin oligomerizations or polymns. procede via the hydride mechanism. An exception appears to be the selective trimerization of ethylene to 1-hexene with chromium catalysts- a reaction that may soon be an industrial process. However, the mechanism of this important transformation is still largely unclear. Jolly could support a possible mechanism with oxidative addn. of two olefins to a chromium complex giving a metallacyclopentane which inserts a third ethylene to give a metallacycloheptane before .beta.-hydride and reductive elimination regenerates the original complex and 1-hexene. We have found that N-substituted triazacyclohexane complexes of CrCl3 react with MAO to give a homogeneous catalyst for the selective trimerization of alpha-olefins. This allows the detailed study of the mechanism by observation of the reaction in the NMR or UV/Vis and by introducing olefinic N-substituents that participate in the initiation and trimerization.

L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS
AN 1997:784429 CAPLUS
DN 127:354654
TI The Chemistry of 1,3,5-Triazacyclohexane Complexes. 7. Synthesis and Characterization of the Cobalt(II) Methoxide Core {Co3(OMe)4}2+
AU **Koehn, Randolph D.; Haufe, Matthias**; Kociok-Koehn, Gabriele; Filippou, Alexander C.
CS Institut fuer Anorganische und Analytische Chemie, Technische Universitaet Berlin, Berlin, D-10623, Germany
SO Inorganic Chemistry (1997), 36(26), 6064-6069
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB The authors report the synthesis and characterization of the 1st .eta.3-1,3,5-trimethyl-1,3,5-triazacyclohexane (Me3TAC) alkoxo complexes. Dehydration of [Co(H2O)6](X)2 with 2,2-dimethoxypropane or HC(OMe)3 and subsequent treatment with Me3TAC gave the methoxo cube fragment clusters [{(Me3TAC)Co}3(OMe)4](X)2 (X = B(C6F5)4 (2a) and B(m-C6H3(CF3)2)4 (2b)). 2A crystallizes as a solvate in the triclinic space group P.hivin.1 (a 13.857(2), b 16.843(3), c 19.318(2) .ANG., .alpha. 79.23(2), .beta. 76.855(13), .gamma. 70.10(2).degree., Z = 2) and solvated 2b in the monoclinic space group P21 (a 12.710(3), b 23.251(3), c 18.702(4) .ANG., .beta. 101.16(2).degree., Z = 2). The cations contain a {Co3(OMe)4} cube fragment core with an .eta.3-Me3TAC bonded to each Co atom. Me3TAC is bonded unsym. due to H-bonding interactions with the anions. This broken symmetry can also be obsd. as solvent-, anion-, and H/D-isotope-dependent splitting of the signals in 1H and 2H NMR. A byproduct of the reaction is the protonated Me3TAC. The analogous monoacid adduct Me3TAC.cntdot.HCl was characterized by x-ray crystallog. (orthorhombic space group Pbca, a 11.0366(9), b 12.2986(6), c 13.9949(7) .ANG., Z = 8).
ST crystal structure cobalt trimethyltriazacyclohexane methoxo trinuclear; structure cobalt trimethyltriazacyclohexane methoxo partial cubane; cobalt trimethyltriazacyclohexane methoxo partial cubane prepn; azacyclohexane cobalt methoxo partial cubane prepn; hydrogen bond cobalt trimethyltriazacyclohexane methoxo trinuclear
IT Bond length
(cobalt-nitrogen; in cobalt trimethyltriazacyclohexane methoxo trinuclear partial cubane)

IT NMR (nuclear magnetic resonance)
(of cobalt trimethyltriazacyclohexane methoxo partial cubane)

IT Hydrogen bond
(of cobalt trimethyltriazacyclohexane methoxo trinuclear partial cubane)

IT Crystal structure
Molecular structure
(of trimethyltriazacyclohexane hydrochloride and its cobalt methoxo trinuclear partial cubane)

IT Cluster compounds
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and hydrogen bonding of cobalt trimethyltriazacyclohexane methoxo partial cubane)

IT 77-76-9, 2,2-Dimethoxypropane
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of cobalt trimethyltriazacyclohexane methoxo partial cubane)

IT 198197-24-9P 198197-26-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of cobalt trimethyltriazacyclohexane methoxo partial cubane)

IT 50-00-0, Formaldehyde, reactions 74-89-5, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of trimethyltriazacyclohexane)

IT 198197-29-4P 198197-33-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and hydrogen bonding of)

IT 198197-22-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and crystal structure and reaction with cobalt aqua complex salts partial cubane)

IT 198197-30-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and mol. structure and hydrogen bonding of)

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 1997:157895 CAPLUS

TI Triazacyclohexane complexes of transition metals for olefin polymerization.

AU Koehn, R. D.; Haufe, M.; Seifert, G.; Kociok-Koehn, G.

CS Inst. f. Anorg. u. Analyt. Chemie, Technische Universitat Berlin, Berlin, D - 10623, Germany

SO Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 (1997), INOR-431 Publisher: American Chemical Society, Washington, D. C. CODEN: 64AOAA

DT Conference; Meeting Abstract

LA English

AB In the search for ancillary ligands enforcing unusual coordination geometries in complexes with potential catalytic activity, we investigated the coordination chem. of N-substituted 1,3,5-triazacyclohexanes (R3TAC). X-ray crystallog. on several complexes has shown that this ligand coordinates facially to a variety of transition metals with N-M-N bite angles of around 60.degree. and severely misdirected nitrogen lone pairs deviating from the direct N-M bond by 25-45.degree.. [(R3TAC)CrCl3] reacts with {MeAlO}.chi. (MAO) to solns. that polymerize ethylene. As a model for the active species we attempted to prep. complexes [(R3TAC)MR]n+. As a first structural model, [(R3TAC)ZnEt]+ was prepd. from ZnEt2 and R3TAC/PhNMe2H+. Several complexes (R3TAC)CrR'3 were prepd. However, we were unable to isolate the desired cationic Cr(III) complexes by protonolysis. Similar Cr(II) complexes were also investigated.

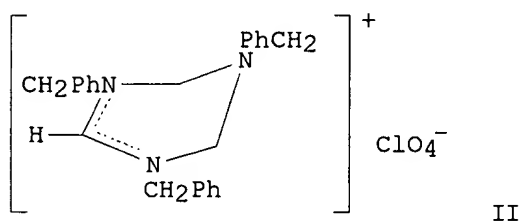
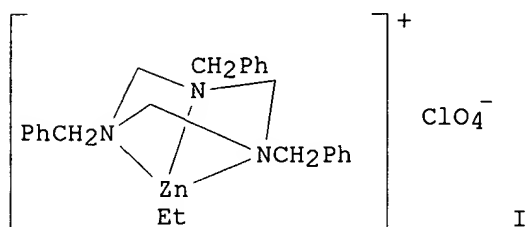
L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 1996:584666 CAPLUS

DN 125:276048

TI The chemistry of 1,3,5-triazacyclohexane complexes. 5. Cationic zinc(II)

alkyl complexes of N-alkylated 1,3,5-triazacyclohexanes and
 13-benzyl-1,5,9-triazatricyclo[7.3.1.0⁵,13]tridecane
 AU **Haufe, Matthias; Koehn, Randolph D.**; Wiemann, Roman;
 Seifert, Guido; Zeigan, Dieter
 CS Institut fuer Anorganische und Analytische Chemie, Technische Universitaet
 Berlin, Berlin, D-10623, Germany
 SO Journal of Organometallic Chemistry (1996), 520(1-2), 121-129
 CODEN: JORCAI; ISSN: 0022-328X
 PB Elsevier
 DT Journal
 LA English
 CC 29-9 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 GI



AB Diethylzinc reacts with hydroperchlorates of N-alkylated
 1,3,5-triazacyclohexanes (R3TAC; R = Me, PhCH₂, iPr) and with the
 hydrotetrafluoroborate of 1,3,5-tris(p-fluorobenzyl)-1,3,5-
 triazacyclohexane (FBz3TAC) to give the corresponding cationic Zn
 complexes [(R3TAC)Zn(Et)][X] (X = ClO₄⁻, BF₄⁻), e.g., I. Similar
 complexes were obtained from diethylzinc treated with [HNMe₂Ph][BF₄] or
 [HNMe₂Ph][B(C₆F₅)₄](Et₂O) in the presence of R4TAC (R = PhCH₂, p-FC₆H₄CH₂,
 S-PhMeCH). The crystal structure of II, a product of the decompn. of I,
 was detd. The structures of [(S-PhMeCH)3TAC]Zn(ET)][BF₄] and
 [(p-FC₆H₄CH₂)3TAC]Zn(ET)][BF₄] were estd. using nuclear Overhauser
 enhancement spectroscopy. Protonolysis of diethylzinc with [HNMe₂Ph][BF₄]
 in the presence of 13-benzyl-1,5,9-triazatricyclo[7.3.1.0⁵,13]tridecane
 (BzTATC) yield [(BzTATC)Zn(ET)][BF₄].
 ST crystal structure triazacyclohexenium; mol structure triazacyclohexenium;
 zinc triazacyclohexane triazatricyclotridecane complex prepn; NOESY
 triazacyclohexane zinc complex; mol mechanics triazacyclohexane zinc
 complex
 IT Crystal structure
 Molecular structure
 (of triazacyclohexenium)
 IT 51720-36-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and crystal structure of)
 IT 118612-00-3P 182175-58-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 108-74-7 121-69-7, N,N-Dimethylaniline, reactions 557-20-0,
 Diethylzinc 2547-66-2 4520-86-9 10556-98-6 131968-96-2
 173449-39-3
 RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotridecane)

IT 22533-76-2P 69737-15-1P 182175-60-6P 182175-65-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotridecane)

IT 182175-68-4P 182175-70-8P 182175-71-9P 182175-72-0P 182175-75-3P 182175-77-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotridecane)

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS
 AN 1996:48776 CAPLUS
 DN 124:276702
 TI The chemistry of 1,3,5-triazacyclohexane complexes. Part 3. High yield synthesis of $[\text{Cr}\{\text{N}(\text{SiMe}_3)_2\}_3]$ and accurate structure determination by cocrystallization with Me_6Si_2
 AU **Koehn, Randolph D.**; Kociok-Koehn, Gabriele; **Haufe, Matthias**
 CS Inst. Anorg. Anal. Chem., Tech. Univ. Berlin, Berlin, D-10623, Germany
 SO Chemische Berichte (1996), 129(1), 25-7
 CODEN: CHBEAM; ISSN: 0009-2940
 PB VCH
 DT Journal
 LA English
 CC 78-5 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 75
 AB The reaction of the $[\text{CrLCl}_3]$ ($\text{L} = \text{N}, \text{N}', \text{N}''$ -trimethyl-1,3,5-triazacyclohexane) with $\text{LiN}(\text{SiMe}_3)_2$ or $\text{NaN}(\text{SiMe}_3)_2$ in petroleum ether yielded nearly quant. $[\text{Cr}\{\text{N}(\text{SiMe}_3)_2\}_3]$ (I) with loss of L. I was crystd. from Me_6Si_2 as $[\text{Cr}\{\text{N}(\text{SiMe}_3)_2\}_3] \cdot (\text{Me}_6\text{Si}_2)_0.5$ which allowed the refinement of the x-ray crystal structure in the trigonal space group $P31c$ (a 16.012, c 8.4796 Å, V = 1882.8 Å³, Z = 2) without severe disorder.
 ST triazacyclohexane chromium complex reaction silylamine; chromium silylamine complex prepn; crystal structure chromium silylamine complex; mol structure chromium trimethylsilylamine complex
 IT Crystal structure
 Molecular structure
 (of chromium bis(trimethylsilyl)amide)
 IT 175285-80-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure; prepn. of bis(trimethylsilylamine) chromium from triazacyclohexane chromium and bis(trimethylsilylamine) lithium)
 IT 175285-79-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (des prepn. of bis(trimethylsilylamine) chromium from triazacyclohexanechromium and bis(trimethylsilylamine) lithium)
 IT 4039-32-1, Lithium Bis(trimethylsilyl)amide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of bis(trimethylsilylamine) chromium from triazacyclohexane chromium and bis(trimethylsilylamine) lithium)

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS
 AN 1995:847433 CAPLUS
 DN 124:56199
 TI .eta.3-1,3,5-Triazacyclohexane complexes of tribenzylchromium(III)
 AU **Koehn, Randolph D.**; Kociok-Koehn, Gabriele; **Haufe, Matthias**
 CS Institut fuer Anorganische und Analytische Chemie, Technische Universitaet Berlin, Strasse des 17, Juni 135, Berlin, D-10623, Germany
 SO Journal of Organometallic Chemistry (1995), 501(1-2), 303-7
 CODEN: JORCAI; ISSN: 0022-328X
 PB Elsevier
 DT Journal

LA English
 CC 29-11 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 AB 1,3,5-Tribenzyl-1,3,5-triazacyclohexane ('Bz3TAC') and
 1,3,5-tricyclohexyl-1,3,5-triazacyclohexane ('Cy3TAC') react with
 CrCl3(THF)3 to the corresponding complexes (Bz3TAC)CrCl3 (1a) and
 (Cy3TAC)CrCl3 (1b). These react with benzylnsodium in toluene to the
 tribenzylchromium(III) complexes (Bz3TAC)Cr(CH2Ph)3 (2a) and
 (Cy3TAC)Cr(CH2Ph)3 (2b). The crystal and mol. structure of
 2b.cntdot.1.5toluene was detd. by x-ray diffraction.
 ST crystal structure chromium benzyl triazacyclohexane complex; mol structure
 chromium benzyl triazacyclohexane complex
 IT Crystal structure
 Molecular structure
 (of chromium benzyl triazacyclohexane complex)
 IT Crystal field theory and Ligand field theory
 (of chromium triazacyclohexane complexes)
 IT Energy level splitting
 (crystal-field, of chromium triazacyclohexane complexes)
 IT 1121-53-5, Benzylnsodium
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for prepn. of chromium benzyl triazacyclohexane complexes)
 IT 2547-66-2, 1,3,5-Tribenzyl-1,3,5-triazacyclohexane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for prepn. of chromium complexes)
 IT 6281-14-7P, 1,3,5-Tricyclohexyl-1,3,5-triazacyclohexane
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (for prepn. of chromium complexes)
 IT 10170-68-0, Trichlorotris(tetrahydrofuran)chromium
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for prepn. of triazacyclohexane complexes)
 IT 108-91-8, Cyclohexylamine, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for prepn. of tricyclohexyltriazacyclohexane)
 IT 172166-81-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and crystal structure of)
 IT 172166-84-6P, Tris(benzyl)(1,3,5-tribenzyl-1,3,5-
 triazacyclohexane)chromium
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and ligand-field parameters)
 IT 172166-82-4P, Trichloro(1,3,5-tribenzyl-1,3,5-triazacyclohexane)chromium
 172166-83-5P, Trichloro(1,3,5-tricyclohexyl-1,3,5-
 triazacyclohexane)chromium
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (prepn., ligand-field parameters and reaction with benzylnsodium)
 IT 172166-80-2P, Tris(benzyl)(1,3,5-tricyclohexyl-1,3,5-
 triazacyclohexane)chromium
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn., mol. structure and ligand-field parameters)

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